

Dimethyl ethylmalonate
26717-67-9 | DTXSID70181214

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -22.9 °C

Global applicability domain: Inside

Local applicability domain index: 8.73e-01

Confidence level: 6.64e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dimethyl glutarate</div> <div>Measured: -42.5</div> <div>Predicted: -25.9</div>	<div>Image not found</div> <div>Diethyl propanedioate</div> <div>Measured: -50.0</div> <div>Predicted: -34.4</div>	<div>Image not found</div> <div>Dimethyl adipate</div> <div>Measured: 10.3</div> <div>Predicted: -9.04</div>
<div>Image not found</div> <div>Diethyl butanedioate</div> <div>Measured: -21.0</div> <div>Predicted: -13.4</div>		